

Controlled multiqubit entangled states and quantum transmission in quantum molecule-spin systems

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Abstract

The multiqubit entangled states are coherently controlled in the quantum spin systems composed of $N + 1$ interacting antiferromagnetic molecular rings. The tunable intermolecular couplings arise from the local exchange interactions between electron spins of N circumjacent magnets and those of one central molecular ring. The quantum dynamics of such system is analytically deduced by the effective spin hamiltonian with anisotropic Heisenberg couplings. It is found that entangled W states can be generated with a high precision under the circumstance of quantum fluctuations. The multiqubit entangled state is also transferred from some molecular rings to others by the selection of intermolecular couplings.

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I. INTRODUCTION

Multiqubit entanglement is identified as a key resource for scalable quantum computation and communication [1, 2]. As an important multiqubit entangled state, an equally weighted superposition of N single-spin state, i.e., the entangled W state, has also been applied to the quantum information processing such as the Grover search [3]. In recent years, the theoretical and experimental constructions of multiqubit entangled states have been demonstrated with very few qubits in nuclear magnetic resonance [4, 5] and trapped ions [6]. However, this result is far away from the scalable quantum information processing in principle. From this point of view, significant efforts have been devoted to the study of quantum dynamics of many spins in quantum dots [7], semiconductors [8] and molecular magnets [9]. Electron spins in these solids are considered among the promising candidates for quantum information technology [10]. Due to the range of neighboring spins in quantum dots and semiconductors, the local control over the electrical and magnetic field is very challenging [11]. This is becoming one main technological obstacle in the implementation of quantum logic gates. In this perspective, single molecular magnets(SMMs) with antiferromagnetic interactions can act as effective qubits [12, 13]. Compared to quantum dots, the molecular and supramolecular chemistry enable the manipulation of long range interactions between coupled molecular rings [14]. Even for the fast control requirement, the preferable electric control over SMMs is also possible [15]. The proposal of quantum gates [16] based on two molecular magnets such as $Cr_xNi(x = 3, 5, 7)$ has been put forward. In the interesting experiment [17], Cr_xNi rings can be linked to each other so conveniently that the effective coupling between them can be chemically tuned by choosing the linker. Therefore, it is very valuable to investigate the multiqubit entanglement in this quantum hardware which consists of a collection of coupled molecular magnets.

In this paper, our attentions are focused on the special quantum systems with N antiferromagnetic molecular rings which are weakly coupled to a central molecular magnetic. In Sec. II, for the typical example of Cr_xNi , the effective spin hamiltonian of $N + 1$ coupled molecular magnets can be obtained in the form of anisotropic Heiserberg exchange. In Sec. III, we analytically give the exact quantum dynamics of the system in the single-spin subspace. The entangled W state is generated in this controllable quantum systems. And the multiqubit entangled states can also be perfectly transmitted from some rings to others by

means of choosing the intermolecular coupling. A useful discussion concludes the paper.

II. EFFECTIVE SPIN HAMILTONIAN OF COUPLED MOLECULAR MAGNETS

Some molecular magnets [18, 19] have been synthesized as suitable candidates for carrying the quantum information and qubit encoding. In particular, a class prototypical system of the substituted antiferromagnetic Cr_xNi rings can act as an effective two-level quantum system at low temperatures and show the long decoherence time. Here, we take into account the quantum systems of $Cr_{x_i}Ni$ rings with the number of N which are weakly coupled to a central molecular ring $Cr_{x_c}Ni$. The hamiltonian of the quantum system can be described as

$$H = H_i + H_c + H_{int} \quad (1)$$

Here H_i and H_c are the spin hamiltonians of the i th circumjacent ring and central one respectively. According to [20], the spin hamiltonian of Cr_xNi is

$$H_x = \sum_{k=1}^{x+1} J_k \vec{\tau}_k \cdot \vec{\tau}_{k+1} + d_k [\tau_{k,z}^2 - s_k(s_k + 1)/3] \\ + \sum_{k \neq l} \vec{\tau}_k \cdot \vec{D}_{k,l} \cdot \vec{\tau}_l, (x = x_i, x_c) \quad (2)$$

where $\vec{\tau}_k$ is the spin operator of the k th electron spin in a molecular ring, $k = x + 1$ describes the site of Ni substitution ($s_{x+1} = 1$) and others denote the sites of Cr irons ($s_k = 3/2$). The first item of the above equation is the dominant isotropic Heisenberg exchange with different couplings $J_{x+1}/J_k = a$, while the second and third ones account for the anisotropic local crystal field and the intramolecular dipolar interaction. For the experimental measurements, the intramolecular dipolar coupling is small enough to be neglected in the following context. With the idea of the local exchange between the m th electron spin in the i th circumjacent ring and the n th one in the central ring, the form of H_{int} is expressed by

$$H_{int} = \sum_{i=1}^N \sum_{(m,n)} J_{m,n}^i \vec{\tau}_m^i \cdot \vec{\tau}_n^c \quad (3)$$

Here, the symbol of $\sum_{(m,n)}$ includes all possible pairs of selective local linkers between two rings where (m, n) denotes one pair. At very low temperatures, all of the antiferromagnetic molecular rings serve as effective qubits for the ground doublet states $\{|0_{i(c)}\rangle, |1_{i(c)}\rangle\}$ with

the total spin $S_{i(c)} = 1/2$. These two degenerate states are separated from the next excited state by a large energy gap Δ_g . For the weak local exchanges, the Heisenberg interaction of H_{int} can be expressed by the effective molecular spin operators $\vec{S}_{i(c)}$

$$H_{int} = \sum_{i=1}^N \frac{\gamma_i}{2} [(S_i^+ S_c^- + S_i^- S_c^+) + (1 + \Delta_i) S_i^z S_c^z] \quad (4)$$

where the effective intermolecular interaction can be described by $\gamma_i \sim \sum_{m,n} J_{m,n}^i \langle 1_i | \tau_m^{i,x} | 0_i \rangle \cdot \langle 0_c | \tau_n^{c,x} | 1_c \rangle$ and the anisotropy $\Delta_i = 1 - \frac{\sum_{m,n} \langle 0_i | \tau_m^{i,z} | 0_i \rangle \cdot \langle 0_c | \tau_n^{c,z} | 0_c \rangle}{\sum_{m,n} \langle 1_i | \tau_m^{i,x} | 0_i \rangle \cdot \langle 0_c | \tau_n^{c,x} | 1_c \rangle}$. It shows that the interactions closely depend on the definite structures of the molecular rings and local linkers. The recent experiment has demonstrated that the effective couplings can be chemically tuned by the control of the local linkers between two molecular rings [?]. Without losing the generality, the controllable anisotropy is calculated for two coupling rings Cr_3Ni with the same structure. It is seen that the anisotropy Δ can be varied with the change of the ratio of the intramolecular couplings a and local crystal field d in Fig. 1(a). When the value of a is near to one, the values of Δ is increased almost linearly with respect to b . By the manipulation of two pairs of local linkers, Fig. 1(b) illustrates that the anisotropy Δ can also be tunable in the large range from the negative value to the positive one. For the special case of $\Delta = -1$, the model of H_{int} is simplified to be the Heisenberg XX one. If the selective local exchanges arrive at a critical ones $b = b_c$, the anisotropy can be rapidly tuned from one negative value to a large positive one. Because of the symmetric property $[H_{int}, \sum_{i=1}^N S_i^z + S_c^z] = 0$, the effective spin Hamiltonian for $N+1$ interacting molecular rings can be described in the single-spin subspace of $\{|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_N\rangle, |\psi_{N+1}\rangle\}$

$$\begin{aligned} H_{eff} |\psi_i\rangle &= \frac{\gamma_i}{4} [(N-2)(1+\Delta_i) |\psi_i\rangle + 2 |\psi_{N+1}\rangle] \\ H_{eff} |\psi_{N+1}\rangle &= \sum_{i=1}^N \frac{\gamma_i}{4} [2 |\psi_i\rangle - (1+\Delta_i) |\psi_{N+1}\rangle] \end{aligned} \quad (5)$$

where the basis of the subspace $|\psi_i\rangle = |1_i\rangle \otimes \prod_{k \neq i} |0_k\rangle$. At very low temperatures, the quantum information could be processed in this subspace. Then, the dynamics of these states can be analytically solved as follows.

III. GENERATION AND TRANSMISSION OF MULTIQUBIT ENTANGLED STATES

Our quantum memory registers will be expanded by the set of states in the single-spin subspace for low temperatures $k_B T \leq \Delta_g$. The general expression of the effective Hamiltonian H_{eff} can be obtained

$$H_{eff} = \frac{1}{4} \begin{pmatrix} \gamma_1(1 + \Delta_1)(N - 2) & 0 & \cdots & 0 & 2\gamma_1 \\ 0 & \gamma_2(1 + \Delta_2)(N - 2) & \cdots & 0 & 2\gamma_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \gamma_N(1 + \Delta_N)(N - 2) & 2\gamma_N \\ 2\gamma_1 & 2\gamma_2 & \cdots & 2\gamma_N & -\sum_i^N \gamma_i(1 + \Delta_i) \end{pmatrix} \quad (6)$$

By means of the tunable exchanges $J_{m,n}^i$ for the local selective linkers, the anisotropic interactions can be controlled and satisfy $\gamma_i(1 + \Delta_i) = C$. In this condition, we can analytically obtain the eigenstates and corresponding eigenvalues. The effective Hamiltonian H_{eff} has $N - 1$ degenerate states $|\phi_i\rangle$ with the same eigenvalue $\lambda_i = \frac{C(N-2)}{4}$ and two nondegenerate states $|\phi_j\rangle (j = N, N + 1)$ with $\lambda_{N,N+1} = \frac{1}{4}[-C \pm \sqrt{4\Omega^2 + C^2(N - 1)^2}]$ where $\Omega = \sqrt{\sum_i^N \gamma_i^2}$. The set of all orthonormalized eigenstates can be given by

$$\begin{aligned} |\phi_i\rangle &= \frac{1}{\Gamma_i \Gamma_{i+1}} (\gamma_1 \gamma_{i+1}, \dots, \gamma_i \gamma_{i+1}, -\Gamma_i^2, 0, \dots, 0)^T \\ |\phi_j\rangle &= \frac{X_j}{\Gamma_N} (\gamma_1, \dots, \gamma_N, Y_j \Gamma_N / X_j)^T, (j = N, N + 1) \end{aligned} \quad (7)$$

where the parameters $\Gamma_i = \frac{2\sqrt{\sum_k^i \gamma_k^2}}{C(N-2)}$ and $X_j = \frac{1}{\sqrt{1 + (\lambda_j - 1)^2 / \Gamma_N^2}}$, $Y_j / X_j = \frac{\lambda_j - 1}{\Gamma_j}$ ($j = N, N + 1$). To study how to generate the multiqubit entangled states, we need to find the evolution operator in the single-spin subspace

$$U(t) = \sum_k^{N+1} \Lambda_k(t) |\phi_k\rangle \langle \phi_k| \quad (8)$$

where $\Lambda_k = \Lambda = \exp(-i \int_0^t \frac{C(N-2)}{4} d\tau)$, ($k \neq N, N + 1$) and $\Lambda_{N,N+1} = \exp(-i \int_0^t \lambda_{N,N+1} d\tau)$.

For illustration, we choose two kind of typical initial states. If the initialized state is $|\Psi(0)\rangle = |\psi_i\rangle_{i \neq N+1}$, the general state at any time t is obtained by

$$|\Psi(t)\rangle = \sum_{m \neq i} \frac{\gamma_m \gamma_i}{\Omega^2} (R - \Lambda) |\psi_m\rangle + \frac{\gamma_i}{\Omega} S |\psi_{N+1}\rangle + [\Lambda - \frac{\gamma_i^2}{\Omega^2} (\Lambda - R)] |\psi_i\rangle \quad (9)$$

Here $R = \frac{\Lambda}{1+A^2}(e^{i\theta_1} + A^2 e^{-i\theta_2})$, $S = -\frac{A\Lambda}{1+A^2}(e^{i\theta_1} - e^{-i\theta_2})$ and $A = \frac{C(N-1)}{2\Omega} - \sqrt{1 + \frac{C^2(N-1)^2}{4\Omega^2}}$ where the phase angles $\theta_1 = \int_0^t \frac{\Omega A}{2} d\tau$ and $\theta_2 = \int_0^t \frac{\Omega}{2A} d\tau$. At a certain time for $\theta_1 + \theta_2 = \int \frac{\Omega(A^2+1)}{2A} = \pm 2k\pi$ ($k = 0, 1, 2, \dots$), the possibility of $|\psi_{N+1}\rangle$ is zero. For the circumjacent N sites, we need the possibility of each $|\psi_m\rangle_{m \neq i}$ is equal and the ratio of the effective interactions $p = \gamma_m^2 / \gamma_i^2$

$$p = \frac{1 - N \cos \theta_1 \pm \sqrt{2N(1 - \cos \theta_1) - N^2 \sin^2 \theta_1}}{(N-1)^2} \quad (10)$$

The actual quantum state at this time is $|\Psi\rangle = \frac{1}{\sqrt{N}}(\sum_{m \neq i} |\psi_m\rangle + e^{ix} |\psi_i\rangle)$. Then by means of the single-qubit phase operator at the i -th ring, we can obtain the perfect W state. When another initial state is chosen as $|\psi_{N+1}\rangle$, the general state at time t is expressed by

$$|\Psi\rangle = \sum_m \frac{\gamma_m}{\Omega} S |\psi_m\rangle + \frac{\Lambda(A^2 e^{i\theta_1} + e^{-i\theta_2})}{1 + A^2} |\psi_{N+1}\rangle \quad (11)$$

Through the calculation of the possibilities of the eigenstates, it is found out that the entangled W state $|\Psi_W\rangle = \frac{1}{\sqrt{N}} \sum_m |\psi_m\rangle$ can be generated when the time satisfies $\theta_1 + \theta_2 = \pm(2k+1)\pi$, $\Delta = -1$ and $\gamma_m = \gamma$. However, in realistic quantum control, certain fluctuations from internal and external impacts are unavoidable. To evaluate the effects of quantum fluctuation on the generation of the multiqubit entangled state, we take into account the simplest case of $N = 3$ under the circumstance of $|\Psi(0)\rangle = |\psi_3\rangle$ and $\gamma_1 = \gamma_2$. In accordance with the above analysis, the perfect entangled W state can be produced at the time $t_W = 2|k|\pi/\sqrt{C^2 + \Omega^2}$. In regard to the certain fluctuation, the effective intermolecular interactions possibly obey the relation of $\gamma_3(1 + \Delta_3) = C(1 + \delta) \neq \gamma_{1(2)}(1 + \Delta_{1(2)}) = C$. From Fig. 2, it is seen that the error of generation $E_r = 1 - |\langle \Psi_W | \Psi(t_W) \rangle|^2$ is almost linearly decreased with the fluctuation parameter δ . The relation of the values $E_r \sim |\delta|/10$ can demonstrate that the proficiency of the generation of the multiqubit entangled state is high enough to resist the fluctuation to a certain extent.

In solid state quantum computers, it is very necessary to investigate the quantum transport of the multiqubit states. Here we provide a efficient scheme of transferring L -qubit entangled states in our quantum memory registers. For low temperatures, the initial L -qubit entangled state for $L \leq \frac{N-1}{2}$ can be expanded in the single-spin subspace $|\Phi(0)\rangle = \sum_{i=1}^L c_i |\psi_i\rangle$, ($\sum |c_i|^2 = 1$). For the perfect quantum transmission, the entangled state can occur at another L sites from the $L+1$ -th ring to $2L$ -th one after the time. By the analytical calculation, it is found out that the perfect quantum transfer can be achieved in the condition of

$$\frac{\gamma_i}{\gamma_j} = \frac{c_i}{c_j} = \frac{\gamma_{L+i}}{\gamma_{L+j}}, \gamma_{m>2L} = 0 \quad (12)$$

This means that the L -qubit entangled state can be transported perfectly by the adjustment of the effective intermolecular interactions. For an example of $N = 5$, the transferred state is $|\Phi(0)\rangle = \sin \alpha |\psi_1\rangle + \cos \alpha |\psi_2\rangle$ where the two-qubit entangled state $(\sin \alpha |10\rangle_{1,2} + \cos \alpha |01\rangle_{1,2})$ exists in two rings of $i = 1, 2$. To access the quantum transfer in this system, the fidelity at time t is used in the form of

$$F = |\langle \Phi(t) | \Phi(0) \rangle|^2 \quad (13)$$

It is seen that the values of fidelity take on the periodic evolution with the time in Fig. 3. The perfect quantum transmission can be realized by the efficient manipulation of the effective intermolecular couplings.

IV. DISCUSSION

The multiqubit entangled W state can be generated by chemically tuning the effective intermolecular interactions in the quantum system of $N+1$ weakly coupled antiferromagnetic molecular rings. This method can provide an important entanglement source for the scalable quantum search in solids. In the present work, the anisotropy of the effective spin Hamiltonian can be chemically controlled by the selection of local linkers between electron spins of different rings. For low temperatures, the state carrying quantum information can be expanded in the single-spin subspace. The high precision of producing W state at N circumjacent rings can be satisfied with the consideration of a certain fluctuations. And the L -qubit entangled state can also be perfectly transferred at a series of periodic time in our quantum registers by means of the control of the effective long range couplings between

molecular rings. This is also an efficient proposal for the quantum router [21] in which the communication can be directed between any chosen rings.

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Figure caption

Figure 1

(a). The anisotropy Δ is plotted as functions of the ratio of the intramolecular couplings a and local crystal field d for $J_k = 17$; (b). The anisotropy Δ is tuned by the control of two pairs of linkers $b = J_{4,4}/J_{1,2}$ for $J_{1,2} = 1$, $J_k = 17$, $a = 0.9$ and $d = 0.3$.

Figure 2

The error E_r for the generation of W state is plotted as a function of the fluctuation δ for $\gamma_1 = \gamma_2 = 1$.

Figure 3

The fidelity of the quantum state transfer is plotted with the time for the case of $\alpha = \pi/4$, $\gamma_1/\gamma_2 = \gamma_3/\gamma_4 = 1$ and $\gamma_5 = 0$.





